Insulator-Metal Transition in One Dimension Induced by Long-Range Electronic Interactions

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The effects of a long range electronic potential on a one dimensional commensurate Charge Density Wave (CDW) state are investigated. Using numerical techniques it is shown that a transition to a metallic ground state is reached as the range of the electron-electron repulsion increases. In this metallic state, the optical conductivity exhibits a large Drude weight. Possible interpretations of our results are discussed.

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As the dimensionality of an electronic system decreases, it is expected that charge screening would become less important in effectively reducing the range of the electron-electron interactions. Thus, in one dimension (1D) the long-range (LR) Coulomb potential should play an important role in determining the physical properties of electronic models. [1] Experiments in *GaAs* quantum wires [2] and quasi-one-dimensional conductors [3] indeed highlight the importance of LR interactions between carriers. Recently, the role of a $1/r$ Coulomb repulsion on the long distance properties of electrons confined to a chain has been theoretically investigated using bosonisation techniques [4]. The $4k_F$ charge correlations decay very slowly with distance suggesting that the ground state (GS) is similar to a classical Wigner crystal. However, this previous study was made in the continuum limit and the role of the lattice in this context is unclear. In addition, theoretical [5] and experimental [6] results suggest that Umklapp processes have a crucial importance in 1D close to the Mott transition.

In order to investigate the interplay between the Coulomb interaction and Umklapp scattering on the phase diagram and transport properties of 1D systems, here static and dynamical observables are calculated on chains with a variety of electron-electron interactions using numerical techniques. As the range of the electronic potential increases, an insulator to metal transition occurs. In particular, for unscreened $1/r$ Coulomb interactions on a lattice our computational analysis suggests that the GS is *metallic*, an interesting result considering that for short-range interactions (SR) and the densities studied here the GS is a CDW insulator.

The model analyzed here consists of a single chain with L-sites and an extended Hubbard-like interaction,

$$H = -t \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + h.c.) + \sum_{i \geq j} V_{i-j} (n_i - \bar{n})(n_j - \bar{n}), \quad (1)$$

where n_i ($\bar{n}$) is the local (average) electron density, and the rest of the notation is standard ($t = 1$ is the unit of energy). $V_0 = U/2$ corresponds to the on-site interaction (U is the usual Hubbard local coupling) and will alway be included here. For $|i-j| \geq 1$, three types of potentials will be mainly considered: (i) a plain LR Coulomb interaction $V_{i-j} = V_C/|i-j|$; (ii) a SR potential, typically $V_{i-j} = V_C/|i-j|$ for $|i-j| \leq r_{max}$ and $V_{i-j} = 0$ otherwise, extending up to a distance r_{max} (generally with $r_{max} = r_0 - 1$ where r_0 is the average inter-particle distance, i.e. $r_0 = 1/\bar{n}$ in units of the lattice spacing); and (iii) a "mixed" potential with a Coulomb tail of adjustable intensity, $V_{i-j} = V_C/|i-j|$ for $|i-j| \leq r_{max}$ and $V_{i-j} = \beta V_C/|i-j|$ for $|i-j| > r_{max}$, $0 < \beta < 1$. Using Exact Diagonalization techniques, 1D chains are here analyzed. A uniform ionic background has been included in Eq. (1) such that the electrostatic energy per unit volume remains finite.

Let us start with a purely 1D commensurate CDW insulator (reference state) on which the LR Coulomb tail is switched on. For commensurate densities and with SR interactions, it is well-known that Umklapp processes can lead to an instability of the Luttinger Liquid GS towards an insulating state. [7] Let us explore model Eq.(1) with a SR potential using $r_{max} = r_0 - 1 = 2$ at density $\bar{n} = 1/3$ varying the couplings U and V_C in order to determine a set of parameters for which the insulating nature of the GS can be unambiguously proven. Such insulating phase can be characterized by a vanishing charge stiffness: if the electrons experience a flux Φ (in unit of the flux quantum) threaded through the ring, the GS energy E_0 will become independent of Φ once the chain length exceeds some characteristic localization length. In Fig. 1(a) the charge stiffness $D = \partial^2 (E_0/L)/\partial \kappa^2$ (where $\kappa = \frac{2\pi}{L}\Phi$) is shown

as a function of $1/L^2$ (a scaling behavior also followed by Luttinger Liquid (LL) chains [8]). In the case of the SR potential the data strongly suggests an insulating state since $D \to 0$ when $L \to \infty$ for the couplings chosen here.

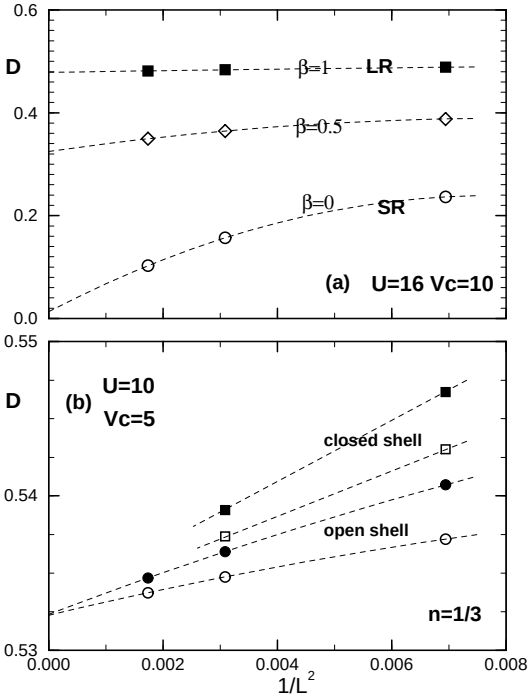

FIG. 1. Charge stiffness D vs $1/L^2$ for $\bar{n} = 1/3$. Dashed lines correspond to polynomial fits of the form $a + b\frac{1}{L^2} + c\frac{1}{L^4}$. (a) Comparison between SR and LR potentials for open shell configurations. The SR potential extends up to $r_{max} = 2$; (b) Comparison between $V_C^{sin}(r)$ (filled symbols) and $1/r$ (open symbols) potentials for boundary conditions giving rise to open or closed shell configurations.

The insulating character of this state can be further established from the finite size scaling behavior of the single particle excitation energy (Fig.2), defined as $\Delta_{C,1}(L) = E_0(\bar{n}L+1, L) + E_0(\bar{n}L-1, L) - 2E_0(\bar{n}L, L)$, where $E_0(N_e, L)$ is the GS energy for N_e electrons and L sites [9]. For the SR potential and the same parameters as previously, Fig. 2(a) strongly suggests that $\Delta_{C,1}$ extrapolates to a finite and sizable gap. In addition, explicitly evaluating real space charge correlations in this state a well-pronounced $4k_F = 2\pi\bar{n}$ pattern was observed. The physical nature of this state is then clear: it forms a commensurate CDW state in which the particles are localized on every r_0 sites. In the thermodynamic limit, the GS is r_0-fold degenerate with gapped charge excitations [10].

Let us now consider a more extended interaction. The $U = \infty$ phase diagram of the repulsive V_1–V_2 model at quarter filling ($\bar{n} = 1/2$) obtained from the investigation of the charge gap $\Delta_{C,1}$ is shown in Fig. 3 (V_1 and V_2 are the electronic density-density repulsion at distance 1 and 2, respectively, while at larger distances the interaction

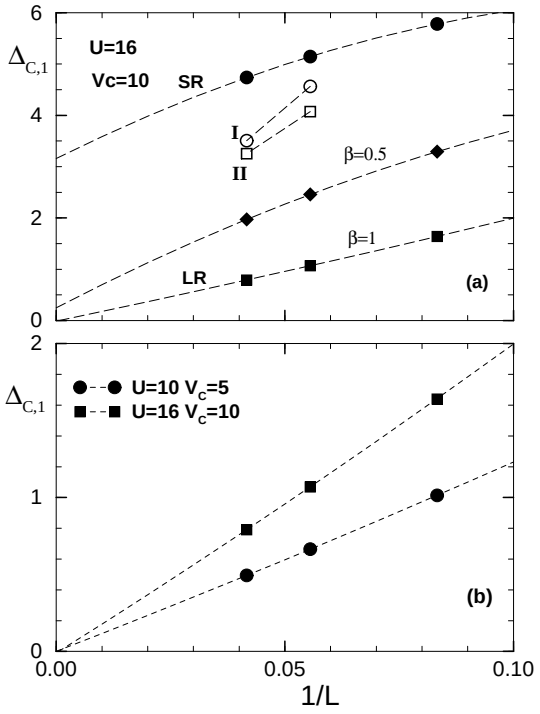

FIG. 2. Finite size scaling of the single particle gap $\Delta_{C,1}$ using $U = 16$ and $V_C = 10$. Dashed lines correspond to polynomial fits of the form $a + b\frac{1}{L} + c\frac{1}{L^2}$. (a) Comparison between SR and Coulomb (LR) interactions. (b) $1/r$ Coulomb potentials. The positions of the absorption peaks labeled by I and II in Fig. 4(b) are also shown (open symbols).

is zero). For such a density ($r_0 = 2$), the line $V_2 = 0$ corresponds to an insulating CDW state above a critical value of V_1 in agreement with our previous results for $\bar{n} = 1/3$, and with earlier calculations using spinless fermions by Emery and Noguera [11]. When a finite V_2 is slowly switched on (now $r_{max} = r_0$) the insulating phase is destroyed above a critical line. Thus, a repulsion beyond distance $r_0 - 1$ drives the system metallic starting from a CDW insulator. Of special importance is the case $V_2 = V_1/2$, which fulfills the relation between the first terms of the Coulomb interaction, since it corresponds to a particularly stable metallic GS. It is also important to stress that the metallic state is here of the Luttinger Liquid (LL) type with $\omega_\rho(q) \sim u_\rho q$ charge excitations. The corresponding values of the LL exponent α characterizing the density of states [3] ($N(\omega) \sim \omega^\alpha$) are shown on Fig.3. This exponent was obtained using $\alpha = (K_\rho + K_\rho^{-1} - 2)/4$, and K_ρ was calculated from the compressibility and the charge velocity following a standard procedure. [12]

Let us now turn to the case of a $1/r$ Coulomb potential. To facilitate the comparison with the previous results for the CDW insulating regime, the density $\bar{n} = 1/3$ at $U = 16$ and $V_C = 10$ will be considered. When the LR tail is added, in contrast to the SR potential, the scaling of the charge stiffness in Fig. 1(a) suggests that it

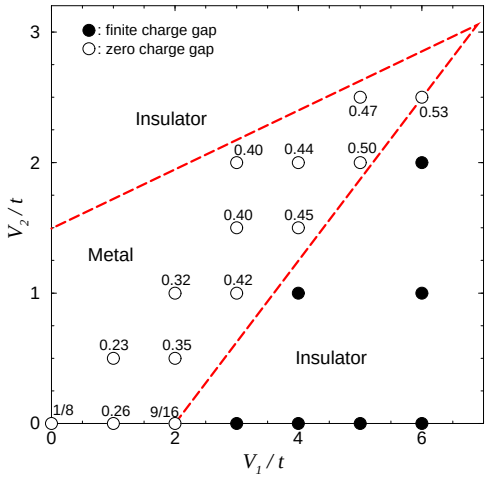

FIG. 3. Phase diagram of the V_1-V_2 model ($U = \infty$) at a density of $\bar{n} = 1/2$. See also Ref. [11]. The extrapolated values of the exponent α are indicated on the plot.

reaches a finite value as $L \to \infty$. To check the accuracy of the finite size extrapolation the sine approximation to the Coulomb potential $V_C^{sin}(r) = \frac{V_C}{\pi L}/\sin(r/\pi L)$ was also considered. A comparison between V_C^{sin} and the plain $1/r$ interaction is shown in Fig. 1(b). All data sets are consistent with the same bulk extrapolation. Then, the present results show that the commensurate CDW state undergoes a transition to a metallic state as the range of the electronic interaction grows.

The metallic character of the $1/r$ Coulomb model can also be further established from the finite size scaling of the single particle gap $\Delta_{C,1}$ as shown in Figs. 2(a,b). For the sets of parameters considered here, a robust $1/L$ scaling behavior is found which suggests that the charge gap vanishes in the bulk, consistent with the finite value of the charge stiffness found before. It is interesting to observe that using a weaker Coulomb tail of amplitude βV_c ($\beta < 1$) also drives the system into a metallic state as shown for $\beta = 0.5$ in Figs. 1(a) and 2(a). This suggests that the range of the interaction, rather than its intensity, is the key element in inducing the insulator-metal transition. Also note that the model with LR interactions is metallic apparently at any value of V_C/t, i.e. an infinitesimal amount of kinetic energy is enough to destroy the insulating state. This is to be contrasted with SR models, such as the $t-V_1$ model, where an insulator-metal transition occurs only for a large enough hopping amplitude [11]. In addition, the metallic state exhibits collective spin modes similar to those of a LL, i.e. with a dispersion $\omega_\sigma(q) \sim u_\sigma q$. Using finite size chains u_σ can be easily calculated on closed shell configurations for $L = 12$, 18 and 24 sites, by means of the energy difference between the first triplet state with momentum $2\pi/L$ and the GS. We have found that u_σ follows very closely a $1/L^2$ scaling behavior, which enables an accurate determination of its bulk value (table I). The small values of u_σ indicates that the effective exchange coupling between neighboring particles at a distance r_0 is small.

To gain insights on the transport properties of the metallic state observed here, the zero-temperature optical conductivity

$$\sigma(\omega, T=0) = \pi D\ \delta(\omega) + \sigma_{reg}(\omega), \qquad (2)$$

was numerically investigated. Results for the LR potential are shown in Fig. 4(a) for $L = 18$ and $L = 24$ rings. The shape, as well as the magnitude of the absorption curve, depends weakly on the system size. By calculating separately $\sigma_{reg}(\omega)$, and using the previous results for the charge stiffness D, it can be explicitly checked the validity of the optical sum rule $\pi D/2 + I_0 = \frac{\pi}{2} E_K^0/L$, where E_K^0/L is the kinetic energy per site and I_0 is the finite frequency integrated absorption. Extrapolations ($L \to \infty$) of these quantities are provided in Table I. It is clear that the metallic and insulating regimes have very different transport properties. Specially, the weight of the absorption band of the metallic state (given by $\sigma_{reg}(\omega)$) corresponds only to 1 to 2% of the total weight, while it exhausts the total sum rule in the case of the insulator [13]. On the other hand, the energy scales of the absorption bands are comparable for the insulator and the metal (Fig. 4(b)). With increasing system size the largest low energy peak in $\sigma_{reg}(\omega)$ shifts to lower energy (see a comparison with $\Delta_{C,1}$ in Fig. 2) as its weight decreases. These excitations might correspond to excitons which have lower energies than the CDW gap when finite range interactions are considered.

A simple interpretation of the insulator-metal transition observed here is as follows: consider the potential experienced by a mobile electron on a chain assuming the rest of the electrons are fixed into a CDW configuration, with particles equally spaced at distances $r_0 = 1/\bar{n}$. For a strong SR interaction the mobile electron is trapped in a deep square-well potential, compatible with the insulating properties observed numerically. However, as the potential range increases the potential experienced by the mobile electron diminishes. Actually, in the (unphysical) limit where the repulsive potential between electrons is made distance-independent such potential becomes irrelevant. This "one-electron" interpretation is favored by the fact that the insulator-metal transition is not associated only with the (usually subtle) $1/r$ interactions but it appears also for the SR $V_1 - V_2$ model as well (Fig. 3).

An alternative interpretation of our results involves a transition from a pinned CDW to a Wigner crystal driven by the LR part of the potential [14]. The bosonisation calculations suggest that the low frequency, long wavelength conductivity of the Wigner crystal should behave as [7],

$$\sigma(\omega, q) \propto \frac{i(\omega + i\epsilon)}{(\omega + i\epsilon)^2 - (\omega_\rho(q))^2}\ . \qquad (3)$$

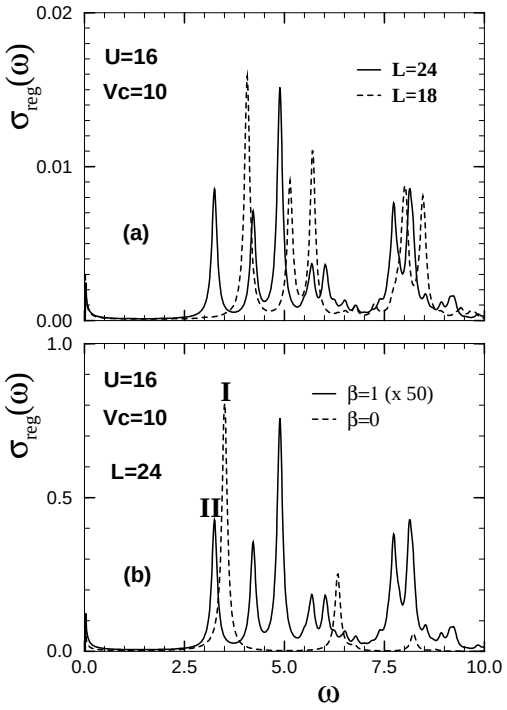

FIG. 4. Optical absorption of a $1/r$-Hubbard chain. (a) Data for 18- and 24-sites chains. (b) Comparison with the insulating CDW state ($\beta = 0$). The small absorption in the case of the LR Coulomb potential ($\beta = 1$) has been multiplied by a factor 50 and the comparatively (very) large Drude peak at $\omega = 0$ has been omitted for clarity.

In general, the $q \to 0$ and $\omega \to 0$ limits do not commute. The relations $\sigma(\omega, q = 0) = 2D_{\rm Drude}\delta(\omega)$ and $\sigma(0, q) = G\delta(q)$ define the Drude weight $D_{\rm Drude}$ and the conductance G, respectively. Using $\omega_\rho(q) \propto q|\ln q|^{1/2}$ (plasmons), [4] Eq. (3) leads to a finite Drude weight and a vanishing conductance. The Drude weight is directly related to the charge stiffness calculated previously by $D_{\rm Drude} = \pi D/2$. Therefore, our numerical results for the LR potential on the lattice are also compatible with the bosonisation approach in the continuum limit, suggesting that a metallic Wigner crystal GS can be realized on a lattice. [15] The metallicity is caused by collective excitations in this scenario.

	u_σ	$\pi D/2$	I_0	sum
$U = V_c = 0$	1	1	0	1
$U = 10$, $V_c = 5$ $\beta = 1$	0.13(5)	0.836	0.010(3)	0.846
$U = 16$, $V_c = 10$ $\beta = 1$	0.04(1)	0.752	0.017(1)	0.769
$U = 16$, $V_c = 10$ $\beta = 0$	0.00(0)	0.0	0.43	0.43

TABLE I. Extrapolated values of the spin velocity u_σ, the Drude weight, the integrated optical absorption and the total sum rule for $\bar{n} = 1/3$.

Quasi–1D organic conductors [16] like $(TMTSF)_2PF_6$ are compounds where $1/r$ Coulomb repulsion might play an important role. This is suggested by ab-initio [17] and Hartree Fock-Valence bond [18] quantum chemical calculations. Note also that despite its many successes, the description of quasi-one-dimensional conductors based on the LL approach still faces various problems to provide a consistent explanation of *all* the experimental data such as NMR relaxation rates [19], photoemission [3] and IR absorption [6]. As argued in this paper, a long-distance $1/r$ Coulomb repulsion within the chains is expected to have drastic effects on the transport properties of such 1D systems, and this phenomenon may contribute to a more accurate theoretical description of 1D conductors.

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sulating phase. However, in contrast to the CDW, we expect the charge-charge correlations to vanish at long distance in a WC.
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